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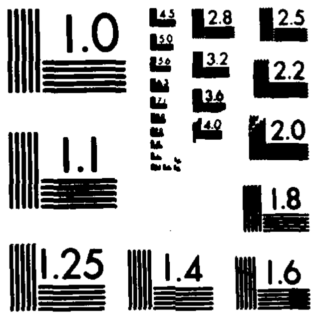

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Period: 1 June 1985 through 31 May 1986

Title of Research: Numerical Methods for Singularly Perturbed Differential Equations with Applications

Principal Investigator: Joseph E. Flaherty

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ABSTRACT

During the period covered by this report we continued our research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We continued our analysis of the stability of mesh moving schemes and developed local refinement and moving mesh schemes for one- and two-dimensional hyperbolic and parabolic problems.

We are applying our methods to several interesting physical problems, such as, elastic-plastic solids, combustion, and a nonlinear Schrodinger equation which exhibits self-focusing. [illegible]

1. Progress and Status of the Research on Adaptive Numerical Methods.

During the past year we concentrated our efforts on developing adaptive finite difference and finite element methods for rather general systems of parabolic and hyperbolic partial differential equations in one- and two-space dimensions. A list of our publications and manuscripts is given in Section 3 of this proposal and herein we will highlight some of our key findings.

Our paper on the stability of several mesh moving schemes that are based on equidistribution appeared in the Journal of Computational Physics [1]. This work explains why some techniques produce grids that either oscillate from time step-to-time step, criss-cross or leave the problem domain. It also suggests strategies for stable mesh motion.

We have extended our mesh moving methods to two space dimensions and a paper describing an algebraic technique by Arney and Flaherty [6] has been accepted for publication. In this approach, a clustering algorithm is used to separate spatially distinct phenomenon and to group regions of high discretization error into rectangles. An algebraic mesh movement function is then used to move and align the mesh with the regions of high error. This procedure is computationally inexpensive, effective, and, unlike many other two-dimensional mesh moving techniques, it has no problem dependent parameters.

Moving mesh methods are effective at following isolated wave fronts, phase boundaries, reaction zones, etc.; however, they have difficulties with intersecting phenomena. Furthermore, no method that uses a fixed number of computational cells can be relied upon to compute solutions to prescribed levels of accuracy. For these reasons, we have been developing techniques that combine mesh moving with local refinement. Our approaches utilize reliable a posteriori estimates of the discretization error to locally add and delete finite difference cells or finite elements as the temporal integration progresses. Thus, they are capable of following and resolving fine scale structures and computing solutions that satisfy prescribed accuracy requirements. Scientists and engineers need not know the proper mesh to use and need only describe their problem in mathematical terms and select appropriate error tolerances. Additionally, since fine discretizations are only used in regions where the solution is varying rapidly, the adaptive software can dramatically reduce computer memory and/or time requirements while providing a measure of confidence in the computed results.

One of our techniques for parabolic systems is a moving method of lines approach with refinement (cf. Adjerid and Flaherty [3, 5]). An estimate of the spatial component of the discretization error is used to move a finite element mesh so as to approximately equidistribute the local spatial discretization error and to recursively add and delete finite elements. The error estimate is obtained by adding a

piecewise quadratic correction to the piecewise linear finite element solution. The superconvergence property of finite element methods for parabolic systems is used to neglect the error at nodes and increase the computational efficiency of the procedure. The finite element solution, error estimation, and refinement algorithms have been extended to two-dimensional parabolic systems (cf. Adjerid and Flaherty [8]) and applied to some difficult combustion problems. A dynamic tree structure is used to efficiently represent the data that is associated with the refinement process. We have proven that our error estimate converges to the true error as the mesh is refined and are writing a paper [10] on our results.

Our method of lines approach couples mesh motion to the solution and error estimate. This produces a method with great stability; however, there are many instances where the extra computational effort is not necessary. For this reason, we have been considering adaptive finite difference and finite element methods that locally refine the mesh in both space and time. Solutions are initially generated on a course grid for one time step. The discretization error at the end of the time step is estimated, finer space-time subgrids are added to regions of high error, and the problem is recursively solved again on the finer grids.. The process terminates and the integration continues to the next time step when the estimated error at the end of the initial time step satisfies a prescribed tolerance. Our progress on a one-dimensional finite element method that uses uniform rectangular space-time grids

appeared in a text on adaptive methods (cf. Bieterman. Flaherty, and Moore [2]). This paper contains some comparisons of our local refinement method with a finite element method of lines due to Bieterman and Babuska. We have also developed a local refinement finite volume code for two-dimensional initial-boundary value problems (cf. Arney and Flaherty [9]). We have combined this refinement technique with the mesh moving technique of [6]. In this approach, a course mesh is moved and finer space-time grids are recursively added to the coarse mesh in regions where greater resolution is needed. The fine grids are properly nested within coarse mesh boundaries: thus. reducing interpolation difficulties at coarse mesh-fine mesh interfaces. Our findings on this technique are being incorporated into a paper [11] that will be submitted for publication shortly.

We are extending our adaptive software and methodologies to include enhancements and improvements. such as. higher order polynomial approximations. special upwind approximations for singularly perturbed problems. combined h- and p-version finite element refinement. techniques for non-rectangular two-dimensional regions. and faster linear algebraic (e.g.. conjugate gradient and multigrid) techniques for our implicit methods. Initially. we will continue investigating one- and two-dimensional problems: however. these areas are fairly well developed and it will soon be possible to consider adaptive techniques for three-dimensional problems. This will necessitate the use of parallel and vector computers. We have been

developing parallel versions of our refinement, solution, and error estimation algorithms and will begin running them on our Sequent systems shortly. We have also extended our piecewise bilinear finite element methods to include piecewise biquadratic approximations. The error of the biquadratic finite element solution can be estimated by local bicubic functions, which only require trivial modifications to our tree data structure. We hope to report our findings at a conference honoring Ivo Babuska at the University of Maryland this Fall.

2. Interactions

Professor Flaherty, Dr. Adjerid, and graduate students supported by this grant lectured and/or visited the following conferences and organizations during the period covered by this report:

J. E. Flaherty visited Los Alamos National Laboratory, 20-21 June 1985 and lectured on "Adaptive numerical methods for time-dependent partial differential equations." He had discussions with Drs. J. M. Hyman, T. Manteufel, B. Swartz, B. Wendroff, and others.

J. E. Flaherty presented an invited lecture on "Local refinement and moving finite element methods for parabolic partial differential equations," at the ASME Applied Mechanics Conference, Albuquerque, NM, 24-26 June 1985.

J. E. Flaherty co-organized (with D. A. Drew) the conference on Mathematics Applied to Fluid Dynamics and Stability which was held at RPI, 9-11 September 1985.

J. E. Flaherty lectured on "Adaptive numerical methods for time-dependent partial differential equations." at the IBM T. J. Watson Research Center, Yorktown Heights, NY, 9 October 1985.

J. E. Flaherty lectured on "Adaptive numerical methods for time-dependent partial differential equations." at the Courant Institute of Mathematical Sciences, New York University, New York, NY, 18 October 1985.

J. E. Flaherty, S. Adjerid, and P. K. Moore attended the SIAM Conference on Parallel Processing for Scientific Computing at Norfolk, VA, 18-20 November 1985.

J. E. Flaherty, S. Adjerid, and P. K. Moore attended the special RPI-University of Maryland Seminar on Adaptive Methods at the University of Maryland, College Park, MD, 24 January 1986. Each of them presented a lecture on adaptive methods for partial differential equations.

J. E. Flaherty presented a lecture on "Adaptive finite element methods for parabolic systems in one- and two-space dimensions." at the Polytechnic

University, Brooklyn, NY, 17 April 1986.

J. E. Flaherty presented a lecture on "Adaptive finite element methods for parabolic systems in one- and two-space dimensions," at the University of Texas, Austin, TX, 5 May 1986.

J. E. Flaherty presented a lecture on "Adaptive finite element methods for parabolic systems in one- and two-space dimensions," at AT&T's Bell Laboratories, Murray Hill, NJ, 15 May 1986.

J. E. Flaherty and S. Adjerid attended the Fourth Army Conference on Applied Mathematics and Computing at Cornell University, Ithaca, NY, 27-30 May 1986. S. Adjerid lectured on "Adaptive finite element methods for parabolic systems in one- and two-space dimensions."

3. List of Publications and Manuscripts in Preparation

Publications

1. J. M. Coyle, J. E. Flaherty and R. Ludwig, "On the Stability of Mesh Equidistribution Strategies for Time Dependent Partial Differential Equations," *J. Comp. Phys.*, Vol. 62 (1986), pp. 26-39.

2. M. Bieterman, J. E. Flaherty, and P. K. Moore, "Adaptive Refinement Methods for Nonlinear Parabolic Partial Differential Equations," Chapt. 19 in I. Babuska, O. C. Zienkiewicz, J. R. Gago, and E. R. Arantes e Oliveira, Eds.,

Accuracy Estimates and Adaptive Refinements for Finite Element Computations, John Wiley and Sons, Ltd., London, 1986.

In Press

3. J. E. Flaherty and S. Adjerid, "A Moving Mesh Finite Element Method with Local Refinement for Parabolic Partial Differential Equations," *Computer Methods in Applied Mechanics and Engineering*, Vol. 55, pp. 3-26, 1986.

4. M. Slemrod and J. E. Flaherty, "Numerical Integration of a Riemann Problem for a van der Waals Fluid," *Res. Mechanica*, accepted for publication, 1984.

5. S. Adjerid and J. E. Flaherty, "A Moving Finite Element Method with Error Estimation and Refinement for One-Dimensional Time Dependent Partial Differential Equations," *SIAM J. Numer. Anal.*, accepted for publication, 1985.

6. D. C. Arney and J. E. Flaherty, "A Two-Dimensional Mesh Moving Technique for Time Dependent Partial Differential Equations," *J. Comp Phys.*, accepted for publication, 1986.

7. T. L. Jackson and J. E. Flaherty, "A Discontinuous Finite Element Method for Hyperbolic Systems of Conservation Laws," submitted to *SIAM J. Sci. Stat. Comput.*, September 1985.

8. S. Adjerid and J. E. Flaherty, "A Local Refinement Finite Element Method for Two-Dimensional Parabolic Systems," submitted to *SIAM J. Sci. Stat.*

Comput., May 1986.

9. D. C. Arney and J. E. Flaherty, "An Adaptive Local Mesh Refinement Method for Time-Dependent Partial Differential Equations," submitted to *SIAM J. Sci. Stat. Comput.*, July 1986.

In Preparation

10. S. Adjerid and J. E. Flaherty, "Local Refinement Finite Element Methods on Stationary and Moving Meshes for One-Dimensional Parabolic Systems," in preparation for *SIAM J. Numer. Anal.*

11. D. C. Arney and J. E. Flaherty, "An Adaptive Method with with Mesh Moving and Local Mesh Refinement for Time-Dependent Partial Differential Equations," in preparation for *SIAM J. Sci. Stat. Comput.*

ON THE STABILITY OF MESH EQUIDISTRIBUTION STRATEGIES FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We study the stability of several mesh equidistribution schemes for time dependent partial differential equations in one space dimension. The schemes move a finite difference or finite element mesh so that a given quantity is uniform over the domain. We consider mesh moving methods that are based on solving a system of ordinary differential equations for the mesh velocities and show that many of these methods are unstable with respect to an equidistributing mesh when the partial differential system is dissipative. Using linear perturbation techniques, we are able to develop simple criteria for determining the stability of a particular method and show how to construct stable differential systems for the mesh velocities. Several examples illustrating stable and unstable mesh motions are presented.

In **J. Comp. Phys.**, Vol. 62, pp. 26-39, 1986.

ADAPTIVE REFINEMENT METHODS FOR NONLINEAR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We consider two adaptive finite element techniques for parabolic partial differential equations (PDEs) that are based on using error estimates to control mesh refinement. One technique is a method of lines (MOL) approach that uses a Galerkin method to discretize the PDEs in space and implicit multi-step integration in time. Spatial elements are added and deleted in regions of high and low error and are all advanced with the same sequence of varying time steps. The second technique is a local refinement method (LRM) that uses Galerkin approximations in both space and time. Fine grids of space-time elements are added to coarser grids and the problem is recursively solved in regions of high error.

Chapter 19 in **Accuracy Estimates and Adaptivity for Finite Elements**, I. Babuska, O. C. Zienkiewicz, E. Arantes e Oliveira, J. R. Gago and K. Morgan (Eds.) 1986

A MOVING MESH FINITE ELEMENT METHOD WITH LOCAL REFINEMENT FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We discuss a moving mesh finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The system is discretized using piecewise linear finite element approximations in space and a backward difference code for stiff ordinary differential systems in time. A spatial error estimation is calculated using piecewise quadratic approximations that use the superconvergence properties of parabolic systems to gain computational efficiency. The spatial error estimate is used to move and locally refine the finite element mesh in order to equidistribute a measure of the total spatial error and to satisfy a prescribed error tolerance. Ordinary differential equations for the spatial error estimate and the mesh motion are integrated in time using the same backward difference software that is used to determine the numerical solution of the partial differential system.

We present several details of an algorithm that may be used to develop a general purpose finite element code for one-dimensional parabolic partial differential systems. The algorithm combines mesh motion and local refinement in a relatively efficient manner and attempts to eliminate problem-dependent numerical parameters. A variety of examples that motivate our mesh moving strategy and illustrate the performance of our algorithm are presented.

In **Computer Methods in Applied Mechanics and Engineering**, Vol. 55, pp. 3-26, 1986.

NUMERICAL INTEGRATION OF A RIEMANN PROBLEM FOR A VAN DER WAALS FLUID

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ABSTRACT

In two recent papers, Slemrod has suggested that the well known Lax-Friedrichs finite difference method may provide a natural method for the numerical integration of initial value problems with an anomalous equation of state, e.g., a van der Waals fluid. In this note we review these ideas and present the results of a numerical experiment which attempts to simulate the dynamics of a van der Waals like fluid.

To appear in **Res Mechanica**, April 1984.

A MOVING FINITE ELEMENT METHOD WITH ERROR ESTIMATION AND REFINEMENT FOR ONE-DIMENSIONAL TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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Dedicated in Memory of Richard C. DiPrima

ABSTRACT

We discuss a moving finite element method for solving vector systems of time dependent partial differential equations in one space dimension. The mesh is moved so as to equidistribute the spatial component of the discretization error in H^1. We present a method of estimating this error by using p-hierarchic finite elements. The error estimate is also used in an adaptive mesh refinement procedure to give an algorithm that combines mesh movement and refinement. We discretize the partial differential equations in space using a Galerkin procedure with piecewise linear elements to approximate the solution and quadratic elements to estimate the error. A system of ordinary differential equations for mesh velocities are used to control element motions. We use existing software for stiff ordinary differential equations for the temporal integration of the solution, the error estimate, and the mesh motion. Computational results using a code based on our method are presented for several examples.

To appear in **SIAM J. Numer. Anal.**, 1985.

A TWO-DIMENSIONAL MESH MOVING TECHNIQUE FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We discuss an adaptive mesh moving technique that can be used with a finite element difference or finite element scheme to solve initial-boundary value problems for vector systems of partial differential equations in two space dimensions and time. The mesh moving technique is based on an algebraic node movement function determined from the geometry and propagation of regions having significant discretization error indicators. Our procedure is designed to be flexible, so that it can be used with many existing finite difference and finite element methods. To test the mesh moving algorithm, we implemented it in a system code with an initial mesh generator and a MacCormack finite difference scheme on quadrilateral cells for hyperbolic vector systems of conservation laws. Results are presented for several computational examples. The moving mesh scheme reduces dispersive errors near shocks and wave fronts and thereby reduces the grid requirements necessary to compute accurate solutions while increasing computational efficiency.

To appear in **J. Comp. Phys.**, 1986.

A DISCONTINUOUS FINITE ELEMENT METHOD FOR HYPERBOLIC SYSTEMS OF CONSERVATION LAWS

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ABSTRACT

We develop an adaptive finite element method for solving nonlinear hyperbolic systems of conservation laws in one space dimension and time. The method uses discontinuous piecewise linear trial functions and continuous piecewise cubic test functions on a moving mesh of triangular space-time elements. The mesh is moved by a technique that uses a weighted average of the local characteristic speeds to select nodal velocities. We show that discontinuous finite element approximations on a moving mesh have the potential of accurately resolving physical discontinuities in the solution. Several computational examples are presented to illustrate the performance of the method.

Submitted to **SIAM J. Sci. Stat. Comput.**, September 1985.

A LOCAL REFINEMENT FINITE ELEMENT METHOD FOR TWO-DIMENSIONAL PARABOLIC SYSTEMS

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ABSTRACT

We discuss an adaptive local refinement finite element procedure for solving initial-boundary value problems for vector systems of parabolic partial differential equations on two-dimensional rectangular regions. The differential equations are discretized in space using piecewise bilinear finite element approximations. An estimate of the spatial discretization error of the solution is obtained using piecewise cubic polynomials that employ nodal superconvergence to gain computational efficiency. The resulting system of ordinary differential equations for the finite element solution and error estimate are integrated in time using existing software for stiff differential systems. The spatial error estimate is used to locally-refine the finite element mesh in order to satisfy a prescribed error tolerance. We discuss several aspects of the refinement algorithm and the dynamic tree data structure that is used to store the mesh, solution, and error estimate. A code that is based on our methods is applied to several examples in order to demonstrate the effectiveness of our error estimation procedure and adaptive algorithms.

Submitted to **SIAM J. Sci. Stat. Comput.**, May 1986.

AN ADAPTIVE LOCAL MESH REFINEMENT METHOD FOR TIME-DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We discuss an adaptive local mesh refinement procedure for solving time-dependent inititial-boundary value problems for vector systems of partial differential equations on rectangular spatial domains. The method identifies and groups regions of the problem domain having large local error indicators into rectangular clusters. The time step and computational cells within clustered rectangles are recursively divided until a prescribed tolerance is satisfied. The refined meshes are properly nested within coarser mesh boundaries; thus, simplifying the prescription of interface conditions at boundaries between fine and coarse meshes. Our method may be used with several numerical solution strategies and error indicators. The meshes may be nonuniform and either stationary or moving.

Submitted to **SIAM J. Sci. Stat. Comput.**, July 1986.

LOCAL REFINEMENT FINITE ELEMENT METHODS ON STATIONARY AND MOVING MESHES FOR ONE-DIMENSIONAL PARABOLIC SYSTEMS

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ABSTRACT

We discuss adaptive local mesh refinement finite element procedures for solving initial-boundary value problems for vector systems of parabolic partial differential equations in one space dimension. The differential system is discretized in space using piecewise linear finite element approximations. An estimate of the spatial discretization error of the solution is obtained using piecewise quadratic polynomials that employ nodal superconvergence to gain computational efficiency. The spatial error estimate is used to move and locally refine the finite element mesh in order to equidistribute a global measure of the spatial discretization error and to satisfy a prescribed error tolerance. The resulting system of ordinary differential equations for the finite element solution, error estimate, and mesh motion are integrated in time using existing backward difference software for stiff differential systems. We establish the convergence of our spatial error estimate to the exact error for linear systems on stationary meshes. A code that is based on our methods is applied to several examples in order to compare and evaluate the effectiveness of mesh moving in combination with local refinement.

In preparation for **SIAM J. Numer. Anal.**

AN ADAPTIVE METHOD WITH MESH MOVING AND LOCAL MESH REFINEMENT FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

We discuss adaptive mesh moving, static rezone, and local mesh refinement algorithms that can be used with a finite difference or finite element scheme to solve initial-boundary value problems for vector systems of time dependent partial differential equations in two space dimensions. An underlying coarse mesh of quadrilateral cells is moved by a simple algebraic node movement function so as to follow and isolate spatially distinct phenomena. The local mesh refinement method recursively divides cells of the moving coarse mesh within regions of large error until a prescribed tolerance is satisfied. The static rezone procedure is used to avoid severe distortion of the coarse mesh. To test our adaptive algorithms, we implemented them in a system code with an initial mesh generator, a MacCormack finite difference scheme for hyperbolic systems, and a Richardson extrapolation based error estimation procedure. Results are presented for several computational examples.

In preparation for **SIAM J. Sci. Stat. Comput.**

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